Message

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Sent: 4/26/2016 7:09:12 PM
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Subject: STICS: Clearance Completion: #ORD-012021: Identification of Novel Perfluoroalkyl Ether Carboxylic Acids (PFECAs) and Sulfonic Acids (PFESAs) in Natural Waters Using Accurate Mass Time-of-Flight Mass Spectrometry (TOFMS)

The clearance for this Chemical Safety for Sustainability product is complete:

- **Product type, subtype:** Journal Article, Peer Reviewed
- **Product title:** Identification of Novel Perfluoroalkyl Ether Carboxylic Acids (PFECAs) and Sulfonic Acids (PFESAs) in Natural Waters Using Accurate Mass Time-of-Flight Mass Spectrometry (TOFMS)
- **Author(s):** Strynar , M,S. Dagnino,R. McMahen,S. Liang,A. Lindstrom ,E. Andersen,L. McMillian,M. Thurman,I. Ferrer and C. Ball
- **Initiator:** Anita McElroy,ord/nerl/heasd/mdab
- **ORD Tracking Number:** Tracking # ORD-012021
- **Product Description / Abstract:** Recent scientific scrutiny and concerns over exposure, toxicity, and risk have led to international regulatory efforts resulting in the reduction or elimination of certain perfluorinated compounds from various products and waste streams. Some manufacturers have started producing shorter chain per- and polyfluorinated compounds to try to reduce the potential for bioaccumulation in humans and wildlife. Some of these new compounds contain central ether oxygens or other minor modifications of traditional perfluorinated structures. At present, there has been very limited information published on these “replacement chemistries” in the peer-reviewed literature. In this

study we used a time-of-flight mass spectrometry detector (LC-ESI-TOFMS) to identify fluorinated compounds in natural waters collected from locations with historical perfluorinated compound contamination. Our workflow for discovery of chemicals included sequential sampling of surface water for identification of potential sources, nontargeted TOFMS analysis, molecular feature extraction (MFE) of samples, and evaluation of features unique to the sample with source inputs. Specifically, compounds were tentatively identified by (1) accurate mass determination of parent and/or related adducts and fragments from in-source collision-induced dissociation (CID), (2) in-depth evaluation of in-source adducts formed during analysis, and (3) confirmation with authentic standards when available. We observed groups of compounds in homologous series that differed by multiples of CF2 (m/z 49.9968) or CF2O (m/z 65.9917). Compounds in each series were chromatographically separated and had comparable fragments and adducts produced during analysis. We detected 12 novel perfluoroalkyl ether carboxylic and sulfonic acids in surface water in North Carolina, USA using this approach. A key piece of evidence was the discovery of accurate mass in-source n-mer formation (H^+ and Na^+) differing by m/z 21.9819, corresponding to the mass difference between the protonated and sodiated dimers.

- **Tracking and Planning**
  - Task: Science, approaches, tools, and data for informing cumulative risk assessment and risk management for high priority classess/groups of chemicals
  - Product: N/A - Not Applicable
  - Project: 4.2: Application, Translation, and Transfer of ORD Science, Data, Tools, Models, and Approaches for Selected Agency Risk Assessment/Management Activities
  - Science Question: How can recent scientific advances help describe human variability, life stages, and population groups?
  - Topic: Cumulative Risk
  - Theme: Cumulative Risk
  - Research Program Area: Chemical Safety for Sustainability

- **HISA? ISI? High Profile?:** Not Applicable
- **QA form attached in STICS?:** No
- **QAPP Reference:** N/A
- **Keywords:**
  - TOFMS
  - high resoluton mass spectrometry
  - novel
  - fluoroether compounds

- **Journal Name:** ENVIRONMENTAL SCIENCE & TECHNOLOGY
- **DOI:** http://dx.doi.org/10.1021/acs.est.5b01215
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